Sulin Liu

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Research Interests

My research focuses on developing deep-learning-enabled probabilistic machine learning and generative modeling for scientific discovery settings. I have been actively working/collaborating with domain scientists on material science problems, such as high entropy alloy modeling and photo-chemical reactions.

Work Experiences

2023 - present	Postdoctoral Researcher, **MIT**	Mentor : Rafael Gómez-Bombarelli
	- Working on ML methods for material science settings	
2021 May-Aug.	Research Intern, **Meta Research**	Mentors : Ben Letham, Eytan Bakshy
	- Developed sparse Bayes optimization for interpretable/simple policy search, resulted in a paper, collaborated with product team and successfully deployed the methods in products	
2015-17	Research Engineer, **Nanyang Technological University, Singapore** Advisor : Sinno Jialin Pan	
	- Conducted research in distributed/federated optimization, multi-task learning	

Education

2017-2023	Ph.D. in Machine Learning, Electrical and Computer Engineering, **Princeton University**
	- Advisors : Ryan P. Adams (CS), Peter J. Ramadge (ECE)
2011-2015	B.Eng. in Electrical Engineering, **National University of Singapore**
	- Minor in Mathematics. Thesis advisor : Cheong Loong Fah
	- Thesis : 3D Scene Reconstruction for Indoor Environment Based on Multiview Homographies
2014	Exchange student, **Georgia Institute of Technology**
	- 9 students selected university wide

Honors and Awards

2023	Schmidt Science Fellows MIT Nomination (Withdrawn)
2022	Princeton ECE Travel Grant Award
2022	NeurIPS Top Reviewer Award, 8%
2020	Azure Cloud Computing Proposal Award, $10,000
2019	NeurIPS Top Reviewer Award, 50%
2018	Anthony Ephremides Fellowship -*awarded to the top first year Ph.D. student in the information science track*
2017	Princeton University Fellowship in Natural Sciences and Engineering -*tuition, fees, stipends*
2017	KDD Conference Travel Award
2014	IEEE Eta Kappa Nu Honor Society

2014	Faculty of Engineering Annual Book Prize -*awarded to student with the best performance in wireless communications*
2013	ST Electronics Book Prize -*awarded to the top sophomore in Electrical Engineering*
2011-15	Singapore Ministry of Education Undergraduate Scholarship -*tuition, fees, stipends*

Publications

Conference papers

2023	**Sulin Liu***(equal contr.), Qing Feng*, David Eriksson*, Benjamin Letham, Eytan Bakshy Sparse Bayesian Optimization, in *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2023. Paper. Code. Video.
2020	**Sulin Liu**, Xingyuan Sun, Peter J. Ramadge, Ryan P. Adams Task-Agnostic Amortized Inference of Gaussian Process Hyperparameters, in *Advances in Neural Information Processing Systems (NeurIPS)*, 2020. Paper. Code. Slides. Video.
2020	Hossein Valavi, **Sulin Liu**, Peter J. Ramadge Revisiting the Landscape of Matrix Factorization, in *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2020. **Oral presentation**. Paper.
2018	Mengchen Zhao, Bo An, Yaodong Yu, **Sulin Liu**, Sinno Jialin Pan Data Poisoning Attacks on Multi-Task Relationship Learning, in *AAAI Conference on Artificial Intelligence (AAAI)*, 2018. Paper.
2017	**Sulin Liu**, Sinno Jialin Pan, Qirong Ho Distributed Multi-task Relationship Learning, in *Conference on Knowledge Discovery and Data Mining (KDD)*, 2017. Paper. Video.
2017	Yaodong Yu*, **Sulin Liu***(equal contr.), Sinno Jialin Pan Communication-Efficient Distributed Primal-Dual Algorithm for Saddle Point Problems, in *Uncertainty in Artificial Intelligence (UAI)*, 2017. Paper.
2017	**Sulin Liu**, Sinno Jialin Pan Adaptive Group Sparse Multi-task Learning via Trace Lasso, in *International Joint Conference on Artificial Intelligence (IJCAI)*, 2017. **Oral presentation**. Paper.

Workshop papers

2023	**Sulin Liu**, Peter J. Ramadge, Ryan P. Adams Generative Marginalization Models, *ICML Workshop on Workshop on Structured Probabilistic Inference & Generative Modeling*, 2023. **Contributed talk, 6/125**. Video.
2022	**Sulin Liu***(equal contr.), Qing Feng*, David Eriksson*, Benjamin Letham, Eytan Bakshy Sparse Bayesian Optimization, in *NeurIPS Workshop on Gaussian Processes, Spatiotemporal Modeling, and Decision-making Systems*, 2022. **Contributed talk, top 5 selected**. Video.
2021	Athindran Ramesh Kumar*, **Sulin Liu***(equal contr., random order), Jaime F. Fisac, Ryan P. Adams, Peter J. Ramadge ProBF : Probabilistic Safety Certificates with Barrier Functions, in *NeurIPS "Safe and Robust Control of Uncertain Systems" Workshop*, 2021

2020	**Sulin Liu**, Xingyuan Sun, Peter J. Ramadge, Ryan P. Adams
	Task-Agnostic Amortized Inference of Gaussian Process Hyperparameters, in *7th ICML Workshop on Automated Machine Learning*, 2020. **Spotlight talk**.

Submitted/working papers

2023	**Sulin Liu**, Peter J. Ramadge, Ryan P. Adams
	Generative Marginalization Models, *Submitted*, 2023. Video.
2023+	Andrew Novick*, **Sulin Liu***(equal contr.), James Damewood, Ryan P. Adams, Rafael Gómez-Bombarelli, Eric Toberer
	Modeling Canonical Ensemble of High-entropy Alloys with Marginalization Networks, *in preparation*, 2023.
2023+	Athindran Ramesh Kumar*, **Sulin Liu***(equal contr., random order), Jaime F. Fisac, Ryan P. Adams, Peter J. Ramadge
	ProBF : Probabilistic Safety Certificates with Barrier Functions, *Preprint*, Paper. Code.

Presentations

Invited and contributed oral presentations

2023	Generative Marginalization Models
	Contributed Talk at ICML Workshop on Workshop on Structured Probabilistic Inference & Generative Modeling, 2023. Video.
2022	Marginalization Networks for Discrete Generative Modeling
	NSF Institute for Data-Driven Dynamical Design Meeting, 2022.
2022	Sparse Bayesian Optimization
	Contributed Talk at NeurIPS Workshop on Gaussian Processes, Spatiotemporal Modeling, and Decision-making Systems, 2022. Video.
2020	Task-Agnostic Amortized Inference of Gaussian Process Hyperparameters
	Spotlight Talk at 7th ICML Workshop on Automated Machine Learning, 2020.
2017	Adaptive Group Sparse Multi-task Learning via Trace Lasso
	International Joint Conference on Artificial Intelligence (IJCAI), 2017.

Selected poster presentations

2020	Task-Agnostic Amortized Inference of Gaussian Process Hyperparameters
	Conference on Neural Information Processing Systems (NeurIPS), 2020.
2017	Distributed Multi-task Relationship Learning
	Conference on Knowledge Discovery and Data Mining (KDD), 2017.

Professional Services

Conference Reviewing

2018-	Conference on Neural Information Processing Systems (NeurIPS)
2019-	International Conference on Machine Learning (ICML)
2020-	Asian Conference on Machine Learning (ACML)
2019-	International Conference on Learning Representations (ICLR)
2021	ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD)
2021	SIAM International Conference on Data Mining (SDM)
2020-2021	AAAI Conference on Artificial Intelligence (AAAI)

Journal Reviewing

2021-	IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)
2020	Journal of Machine Learning Research (JMLR)

Workshop Reviewing

2022	AI for Accelerated Materials Design Workshop, NeurIPS
2022	AI for Science : Progress and Promises Workshop, NeurIPS

Graduate Coursework

- **ML** : Machine Learning and Pattern Recognition, Theoretical Machine Learning, Theoretical Deep Learning

- **Stats** : Statistical Theory and Methods, High-Dimensional Probability, Statistical Optimization and Reinforcement Learning

- **Optimization** : Linear and Nonlinear Optimization, Optimization for Machine Learning, Large-Scale Optimization

- **Control** : Safety-Critical Robotic Systems

Teaching Experiences

Princeton University

2021-2022	Co-instructor for SML 310 Research Projects in Data Science, in Fall 2021 & Spring 2022.
	- Undergraduate project-based course on solving real-world problems with machine learning. Teaching weekly precepts, mentoring students across different disciplines, grading.
2020	Teaching assistant for COS 424 Fundamentals of Machine Learning, in Fall 2020
	- Graduate and undergraduate course on machine learning for large, complex data sets, covering fundamental methods of ML. Teaching precepts, grading, providing feedback to final projects.
2020	Teaching assistant for COS 302 Mathematics for Machine Learning, in Spring 2020
	- Undergraduate course covering mathematics topics (linear algebra, probability, optimization) used in machine learning. Teaching precepts, helping prepare homeworks and exams.
2019	Teaching assistant for SML 201 Introduction to Data Science, in Spring 2019.
	- Undergraduate course covering basic methods and programming of statistics and machine learning. Teaching precepts, programming help-sessions.

2018-2019	Teaching assistant for ELE 535 Machine Learning and Pattern Recognition, in Fall 2018 & Fall 2019 (head TA). - Graduate course covering fundamentals of machine learning, with a focus on theory. Teaching precepts, helping prepare homeworks and exams, grading.

National University of Singapore

2014-2015	Lab tutor for CS 1010E Programming Methodology, in Fall 2014 & Spring 2015. - Undergraduate course covering introductory fundamental concepts of programming. Teaching lab sessions, grading.

Programming Skills

- **Proficient** : Python (PyTorch, Numpy, Pandas), MATLAB, LaTeX, Git, Slurm, Bash/Zsh
- **Familiar** : TensorFlow, C/C++, Java, Parameter Server, HTML/CSS, VHDL

Open Source Projects

Creator and Co-creator :
- AHGP : https://github.com/PrincetonLIPS/AHGP
- ProBF : https://github.com/athindran/ProBF

Developer and Contributor :
- BoTorch : https://github.com/pytorch/botorch
- Ax : https://github.com/facebook/Ax